Relativistic Velocities in Nanomaterials: Analysis of the Diffusion with a new analytical Model

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Abstract — In this paper it is presented the complete technical analysis of the diffusion function in the hypothesis of relativistic velocities inside a nanostructure, considering a current analytical model, which has a wide applicability scale range; we consider in this paper the nanoscale, but a gauge factor inside it permits the application from sub-pico-level to macro-level. Both theoretical framework is performed, and examples of application.


I. INTRODUCTION

Nanomaterials are largely utilized in various applications considering their special properties, which are dependent on size, composition, and structure. The deep understanding of the diffusion process is of great importance for their stability and controlled synthesis. Nanomaterials have unique optical, electronic, magnetic, and chemical properties, which significantly differ from that of their bulk counterparts [1]; these particular properties (higher reactivity, higher saturation magnetization, modified electronic band structures) arise from the fact that they have a large surface-to-volume ratio. Therefore, investigating the local structure of nanomaterials is theoretically and technologically important. Both a need for new techniques probing the diffusion process for nanoparticles and theoretical efforts in the deep comprehension of transport processes are useful and fruitful for improving the innovation in technology. X-rays have been widely utilized in imaging and structure determination of materials, in the range from biomolecules to electronics materials, for its penetrating power and short wavelength. With the synchrotron radiation sources and free electron lasers, progress in X-ray science is fast increasing and new imaging techniques are being realized. The proper understanding of diffusion processes for nanomaterials is important in the synthesis and determination of the material suitability for specific applications, for obtaining desired properties. There are several conventional methods used to study the diffusion in solids (Table I).

<table>
<thead>
<tr>
<th>Indirect Methods</th>
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<tbody>
<tr>
<td>Mechanical spectroscopy</td>
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<td>Magnetic relaxation</td>
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<td>Nuclear magnetic relaxation (NMR)</td>
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<tr>
<td>Impedance spectroscopy (IS)</td>
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<td>Mössbauer spectroscopy (MBS)</td>
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<tr>
<td>Quasi-elastic neutron scattering (QENS)</td>
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<table>
<thead>
<tr>
<th>Direct Methods</th>
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<tbody>
<tr>
<td>Tracer diffusion</td>
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<tr>
<td>Chemical diffusion</td>
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<tr>
<td>Spreading resistance profiling (SRP)</td>
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Table I. Conventional experimental methods for direct and indirect diffusion studies in solids [2].

At the same time, the theoretical study at level of mathematical modelling is essential, considering new models which incorporate the characteristics of the previous ones and offering new peculiarities too. In this paper a recent generalization of the Drude-Lorentz model for transport processes in nanostructures, performed at classical [3] and quantum level [4], is generalized to the case of possible relativistic velocities of carriers inside a nanostructure. The analysis of the function $D(t)$ is considered, completing thus this kind of study together to that performed for the velocities correlation function $\langle \dot{v}(t)\dot{v}(0) \rangle_T$ [5] and the mean square displacement $R^2(t)$ [6].

II. A RECENT ANALYTICAL GENERALIZATION OF THE DRUDE-LORENTZ MODEL

A recent analytical formulation of the Drude-Lorentz model for transport processes shows to fit very well with experimental data and presents interesting new predictions of various peculiarities in nanostructures [7]-[17]. The model studies the dynamics of processes from sub-pico-level to macro-level [18]. It is based on the complete Fourier transform of the frequency-dependent complex conductivity $\sigma(\omega)$, as deduced by linear response theory [19], [20], through a Cauchy integration and the use of residue theorem in the complex plane [21]. The new introduced key idea is the possibility to perform integrations on the entire time axis ($-\infty$, $+\infty$), not only on the half time axis (0, $+\infty$), as usually considered in literature [22], and avoiding time consuming numerical models.
III. EXPRESSION OF THE DIFFUSION FUNCTION FOR RELATIVISTIC VELOCITIES

We consider the possibility of relativistic velocities of carriers inside a nanostructure, studying the condition of relativistic variation of the mass along the $x$-axis on which a nanostructure is placed, in the fixed ground reference frame. About the forces acting on the carrier (electrons in this case, but it is not restrictive), we consider the following outer forces: a passive elastic-type force of the form $F_{rel} = K x$, a passive friction-type force of the form $F_{fr} = \lambda \dot{x}$, with $\lambda = m_{part} / \tau$, and the force deriving by an oscillating electric field $E = e E_0 e^{-i \omega t}$.

Performing the calculation as for the velocities correlation function [5] and the mean square displacement in the relativistic case [6], the analytical expressions of the diffusion function $D(t) = \frac{1}{2} \frac{dR^2(t)}{dt}$ are:

$$\Delta_{rel} > 0$$

$$D(t) = 2 \left( \frac{k_B T}{m_0} \right) \left( \frac{1}{\gamma} \right) \left( \frac{\tau}{\alpha_{rel}} \right) \exp \left( - \frac{t}{2 \tau \rho} \right) \sin \left( \frac{\alpha_{rel} t}{2 \rho \tau} \right),$$

(1)

with $\alpha_{rel} = \sqrt{4 \gamma \omega_0^2 \tau^2 - 1} \in \mathbb{R}^+$;

$$\Delta_{rel} < 0$$

$$D(t) = \frac{k_B T}{m_0} \left( \frac{1}{\tau} \right) \left( \frac{1}{\alpha_{rel}} \right) \times$$

$$\times \left[ \exp \left( \frac{(1 - \alpha_{rel} t)^2}{2 \rho \tau} \right) - \exp \left( \frac{(1 + \alpha_{rel} t)^2}{2 \rho \tau} \right) \right],$$

(2)

with $\alpha_{rel} = \sqrt{1 - 4 \gamma \omega_0^2 \tau^2} \in (0, 1) \subset \mathbb{R}$.

$$\alpha_{rel} / \alpha_{rel} = \sqrt{\Delta_R / \Delta_{rel}},$$

$$\beta = \frac{v}{c},$$

$$\gamma = \sqrt{1 - \beta^2},$$

$$\rho = 1 + \frac{\beta^2}{\gamma^2} = \frac{1}{\gamma^2}.$$

The case $\Delta_{rel} = 0$ reduces to relativistic Drude model.

IV. EXAMPLES OF APPLICATION

As examples of application we considered relativistic velocities of electrons in ZnO nanowires [7], [23], [24]. Changing the nanomaterial, it needs to consider the right effective mass and relaxation time. Moreover, for non-relativistic velocities, the electron rest mass $m_0$ and the effective mass $m_{eff}$ are practically the same. Considered data for Eqs (1,2) are resumed in Table II.

<table>
<thead>
<tr>
<th>$\nu$ (cm/s)</th>
<th>$\beta^2$</th>
<th>$\eta / \rho$</th>
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<tbody>
<tr>
<td>$v_1 = 10^7$</td>
<td>$0.11 \times 10^{14}$</td>
<td>0.998</td>
</tr>
<tr>
<td>$v_2 = 10^8$</td>
<td>0.11</td>
<td>0.888</td>
</tr>
<tr>
<td>$v_3 = 1.5 \times 10^9$</td>
<td>0.25</td>
<td>0.75</td>
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<table>
<thead>
<tr>
<th>$\gamma$</th>
<th>$\tau (s)$</th>
<th>$\omega (s^{-1})$</th>
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<tbody>
<tr>
<td>[23], [24]</td>
<td>$\omega_k, \omega_2, \omega_3$ (fixed)</td>
<td></td>
</tr>
<tr>
<td>1.001</td>
<td>0.28 $10^{-13}$</td>
<td></td>
</tr>
<tr>
<td>1.061</td>
<td>0.28 $10^{-13}$</td>
<td></td>
</tr>
<tr>
<td>1.155</td>
<td>0.28 $10^{-13}$</td>
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Table II. Data utilized in Eqs (1,2); $\omega_k = 10^{12} s^{-1}$, $\omega_2 = 10^{13} s^{-1}$, $\omega_3 = 10^{14} s^{-1}, T = 300 K$.

Figure 1 represents the behavior of $D(t)$ in time for electrons inside a ZnO nanowire [7], [23], [24], considering the parameters: $T = 300 K$, $\tau_1 = 0.28 \times 10^{-13}$ s, $v_1$, $\omega_1$ (red dashed line), $v_2$, $\omega_2$ (green solid line), and $v_3$, $\omega_3$ (blue dot-dashed line).

From Figure 1 we obtain a maximum value of diffusion $D \cong 5 \text{ cm}^2 / \text{s}$ after $t \cong 0.2 \times 10^{-12}$ s. Increasing velocity, we note a decrease in diffusion, as expected considering that the mass increases with $\nu$ (in Eqs (1,2) the mass is at denominator). In Figure 2 we consider ZnO nanowires with the same parameters of Figure 1, with exception of the value of $\omega = \omega_2$. The maximum value of diffusion is $D \cong 4 \text{ cm}^2 / \text{s}$ after $t \cong 0.08 \times 10^{-12}$ s. We note that, in these conditions, the $D$ function decreases more rapidly.

![Figure 1. $D(t)$ vs $t$ for ZnO nanowires; $v_1$, $\omega_1$: red dashed line; $v_2$, $\omega_1$: green solid line; $v_3$, $\omega_1$: blue dot-dashed line.](image)
In this work it has been presented a new result, i.e. the complete analytical form of the function $D(t)$ considering the effect of relativistic velocities of carriers inside a ZnO nanowire. We have utilized a recent new analytical model, appeared both in classical [3] and in quantum form [4], and tested in last years with good accordance with experimental existing data [7]-[16]. Eqs (1,2) return to be those of the classical case [3], when the carriers velocity is classic. The introduced formulae for the diffusion function $D(t)$ complete the version of the model for relativistic velocities of carriers [5], [6]. The considered extension is mathematically very elegant, because of the analytical approach, and can give new interesting information’s, useful in the design phase of new nano-bio-devices with dedicated and specific features. These new information’s may be appropriately tested through experimental time-resolved techniques, like TRTS [25]-[27]

REFERENCES


AUTHOR’S PROFILE

Paolo Di Sia is currently professor of “Foundations of Mathematics and Didactics” at the Free University of Bolzano-Bozen (Italy). He obtained a Degree in Metaphysics, a Degree in Theoretical Physics and a PhD in Mathematical Modelling applied to Nano-Bio-Technologies. He is interested in Classical – Quantum - Relativistic Nanophysics, Theoretical Physics, Planck Scale Physics, Mind-Brain Philosophy, Econophysics and Philosophy of Science. He is author of more than 130 works at today (articles on national and international journals, scientific international book chapters, books, internal academic notes, works on scientific web-pages, in press), reviewer of two mathematics academic books and is preparing a chapter for a scientific international encyclopedia. He is reviewer of some international journals and invited to review and as editor, obtained 4 international awards, included in Who’s Who in the World 2015 (32th edition), member of 5 scientific societies, member of 13 International Advisory/Editorial Boards. 
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